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Simulation approach to weak localization in inhomogeneous two-dimensional systems

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Abstract. A weak localization effect has been studied in macroscopically inhomogeneous 2D system. It is shown, that although the real phase breaking length tends to infinity when the temperature tends to zero, such a system can reveal a saturated behavior of the temperature dependence of that parameter, which is obtained from the standard analysis of the negative magnetoresistance and usually identified by experimenters with the phase braking length.

In recent years, interest to the problem of weak localization is reappeared. One of the reason is that the new experimental results have been obtained. Among them is the saturation of the temperature dependence of the phase breaking length [1]. It causes a storm discussion in the literature (see, e.g., [2] and references therein) and stimulate a new flux of the papers concerning the weak localization.

In order to determine the phase breaking time, a standard fitting procedure is used in most cases: experimental magnetic field dependencies of negative magnetoresistance are fitted to the well-known Hikami expression, the phase breaking length l_φ is used as fitting parameter.

Another approach to the negative magnetoresistance examination is based on analysis of statistics of closed paths [3]. Here, we develop this method and present the results of numerical studies of the negative magnetoresistace due to weak localization in macroscopically inhomogeneous systems. One of possible reasons of the low-temperature saturation of $l_\varphi(T)$ dependence is offered.

1. Main idea

We suppose that an inhomogeneous 2D system consists of a number of puddles which are connected one with other by means of channels (Fig. 1(a)). The transport over puddles and channels is diffusive, i.e. their dimensions are much greater than the mean free path of electrons. In this case a quasi-classical treatment to the problem can be applied. In order to simplify the problem, we believe that the conductance of puddles is much greater than the conductance of channels. Such type of inhomogeneity can be due to inhomogeneous distribution of compensating impurity, for example. It is clear that in this approximation the conductance of 2D system is determined by the conductance of channels, and the interference quantum correction to the conductivity of the system is mainly determined by the closed paths, which starting points lie within the channels. So, if we obtain the area distribution function of the closed paths, which start within the channels, we can calculate the magnetic field dependence of magnetoresistance in such a system.

2. Simulation details

The model inhomogeneous 2D system consists of a number of identical elements connected in series-parallel. Each element includes the channel and parts of puddles. We present the results obtained for two cases: the puddles are connected via long and narrow channels (Fig. 1(b)); and the channels are short and wide (Fig. 1(c)). In simulation, the element is represented as a lattice, the scatterers are placed in a part of lattice sites with the use of a random number generator. A particle starts from some random point within the channel, moves with a constant velocity along straight lines, which happen to be terminated by collisions with the scatterers. After collision it changes the motion direction. If the particle collides with the wells of element, it is reflected specularly. If the particle escapes the channel (shadowed in Fig. 1(c)), it can return back with some probability less than unity (we use the value 0.3). Thereby we specify the kind of inhomogeneity: within the channel the Fermi momentum is less than that in the puddles, that may result from fluctuation of the energy of conduction band bottom. If the particle passes near the starting point at the distance less than $d/2$ (where d is a prescribed value, which is small enough), the path is perceived as being closed. Its length and enclosed algebraic area are calculated and kept in memory. The particle walks over the element until it riches one of the opened ends of the element. As this happens we believe that the particle has left to infinity and will not return. A new start point is chosen and all is repeated.

The parameters used in simulation procedure are following: for the case of long channel, the length and width are equal to 17000 and 400, respectively; for short channel, they are 300 and 2900. The dimensions of each half-puddle are 3000×3000 for both cases. For control, we will present the results obtained for comparably large system with dimensions $10^4 \times 10^4$, which is near-equivalent to the classical infinite 2D system. The density of scatterers fed into simulation gave the mean free path about 40 for all three cases.

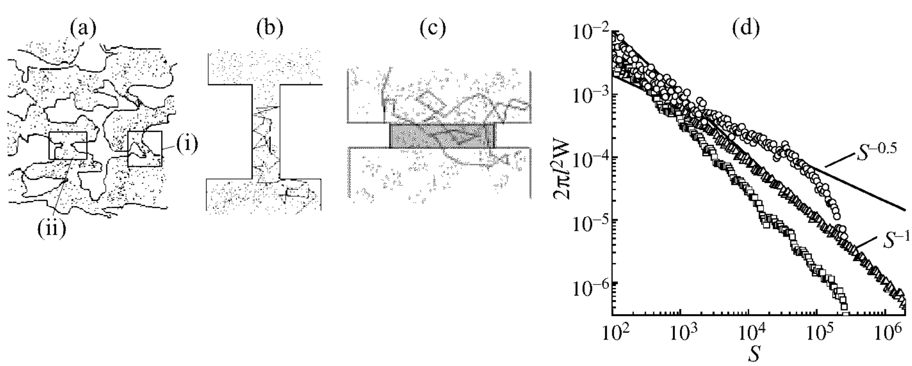

Fig. 1. (a) Sketch of inhomogeneous 2D system. The key parts determining the conductance are enclosed in rectangles. The long and short channels are labeled as (i) and (ii), respectively. Non-conducting areas are white. Points represent scatterers. (b), (c) The simulation models of long and short channels, respectively. Polygonal lines show particle trajectories. The opened ends of shadowed area in (c) work as diode (see text for details). (d) The area distribution function of closed paths. Symbols are the simulation results for the case of long (○), short (□) channels, and for large (control) 2D system (△).

3. Results and discussion

The area distribution functions W, weighted by factor $2\pi l^2$, are shown in Fig. 1(d). As is seen the data obtained for control system and depicted by triangles reveal the behavior which is very close to the well known result of diffusion theory: $2\pi l^2 W = S^{-1}$.

The area dependence of $2\pi l^2 W$ is much complicated for long channels. When S varies within the range $1 \times 10^3 - 5 \times 10^4$, it is close to $S^{-0.5}$-law. Just the same behavior is theoretically predicted for diffusive motion over infinitely long, narrow strip. A particular interest is drastic decrease of the area distribution function evident for $S > 10^5$. The origin is that the particle, moving over long trajectories, escapes the channel through its ends and carries on its motion mainly over the puddles. After escaping it cannot easily enter back, because the width of channel is much less than the puddle's dimensions.

As for short channels, the $2\pi l^2 W$-versus-S plot shows the power behavior close to $W \propto S^{-1.2}$ in whole range of S. This results from the fact that the ratio of the channel's length to the mean free path is not very large as in previous case. Therefore, not only long, but short closed trajectories spread over puddles. Since the channel/puddle borders work as diodes, this leads to more rapid decreasing of $W(S)$ as compared with S^{-1}-law.

The negative magnetoresistance due to magnetic field suppression of the interference quantum correction to the conductivity has been calculated according to [3] and for some l/l_φ value is shown in Fig. 2(a) by symbols. The solid curves in this figure are the results of fitting to the Hikami expression. Namely such a procedure is usually used by experimenters to determine the value of l_φ in real samples. As is seen the Hikami formula well describes the simulation data excepting may be the long channel case.

Figure 2(b) shows the most important result of the paper: how the fitting parameter γ depends on the value of l/l_φ fed into the simulation. As is clearly seen the control 2D system exhibits very clear behavior: as it must the fitting procedure gives the value of γ which is equal to l/l_φ used in simulation. Some inconsistency evident for smallest l/l_φ-value is the result of finiteness of the model system.

For other cases, the fitting procedure gives nearly true value of l/l_φ when $l/l_\varphi >$

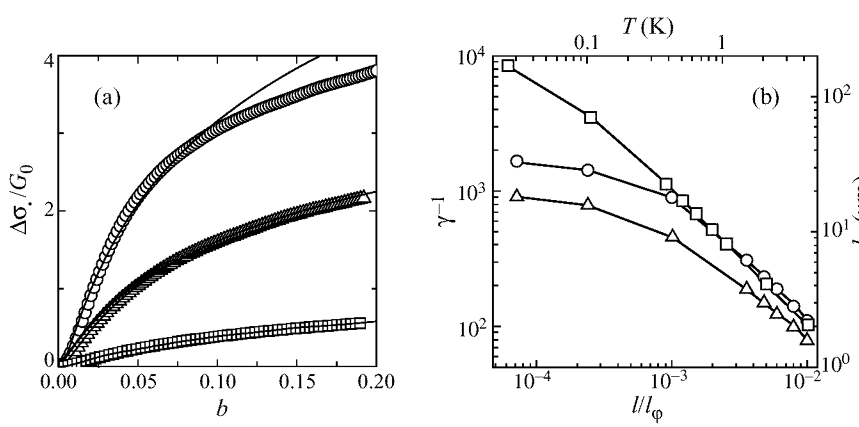

Fig. 2. (a) The magnetic field dependence of interference quantum correction to the conductivity calculated for $l/l_\varphi = 3.5 \times 10^{-3}$. Designations are the same as in Fig. 1(d). Curves are the best fit to the Hikami formula, carried out for low magnetic field $b \leq 0.1$. (b) The fitting parameter γ as function of l to l_φ ratio fed into simulation. Top and right axis give the scale in absolute unites for the 2D system with $n = 1.5 \times 10^{12}$ cm $^{-2}$.

$(2-3)\times10^{-3}$. For lower values of l/l_φ, the γ-versus-l/l_φ plot shows saturation with l/l_φ decreasing. On the assumption of $l_\varphi \propto T^{-1}$ Figure 2(b) shows the temperature dependencies of the "phase breaking length" as it could be found from the standard fitting procedure of negative magnetoresistance to the Hikami expression. In order to specify the scales in Fig. 2(b), let us assume the lattice constant in the simulation to be equal to 5 Å. In this case our model provides an example of 2D system with local density of scatterers 1.5×10^{12} cm^{-2}, mean free path $l = 200$ Å. Then, Fig. 2(b) shows the temperature dependence of the "phase breaking length" for such sample within the temperature range from 25 mK to 4.2 K. Thus, although the real phase breaking length l_φ decreases linearly with decrease of temperature, the value obtained from the fitting procedure is saturated.

4. Conclusion

We have numerically studied the statistics of closed paths and the negative magnetoresistance in macroscopically inhomogeneous 2D systems. It has been shown that such systems can exhibit saturated behavior of the temperature dependence of the "phase breaking length", if it is obtained from the standard fitting procedure of experimental magnetic field dependence of the negative magnetoresistance to the Hikami expression. This fitting parameter can have nothing in common with the real value of phase breaking length at low temperatures.

Acknowledgments

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